



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GOS  
Title : HUMAN MONOAMINE OXIDASE B  
Authors : Binda, C.; Newton-Vinson, P.; Hubalek, F.; Edmondson, D.E.; Mattevi, A.  
Deposited on : 2001-10-26  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

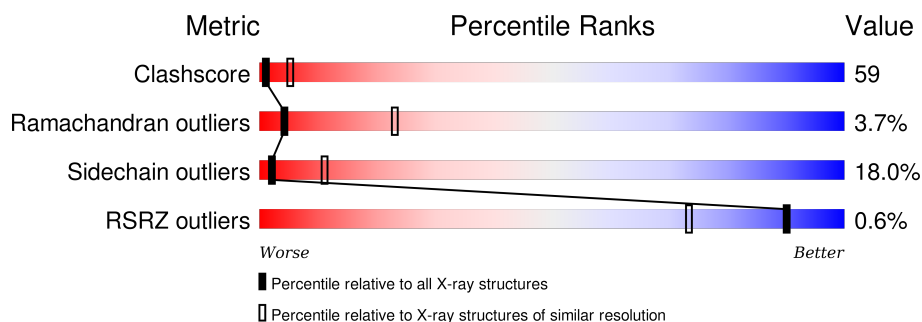
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

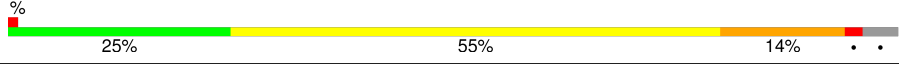

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	
1	B	520	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NYP	A	601	X	-	X	X
3	NYP	B	601	X	-	X	-

## 2 Entry composition [i](#)

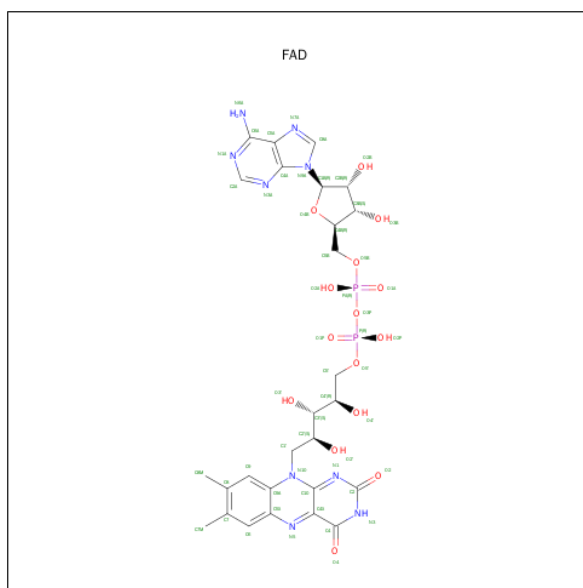
There are 3 unique types of molecules in this entry. The entry contains 8020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MONOAMINE OXIDASE.

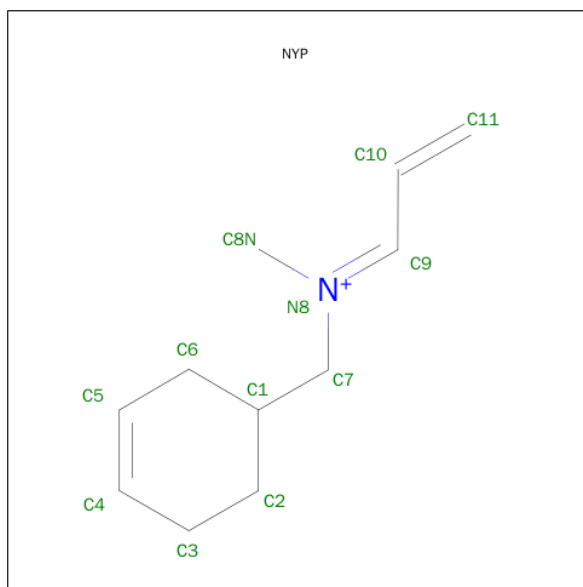
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	B	493	Total	C	N	O	S	0	0	0
			3932	2515	674	719	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-[(E)-METHYL](PHENYL)-N-[(E)-2-PROPENYLIDENE]METHANAMINIUM (three-letter code: NYP) (formula:  $C_{11}H_{18}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	11	1		
3	B	1	Total	C	N	0	0
			12	11	1		



T479	E142	R208	L345	R415	G156	H178	G194
T480	W143	K209	A346	Q416	E179	E179	G194
F481	D144	P210	R347	Q417	W180	W180	T195
L482	N145	F211	K348	V418	S181	S181	T196
E483	N146	Q212	A349	D419	A182	A182	R197
R484	T147	G215	R350	R420	L183	L183	I198
H485	N148	Q216	K351	I421	W184	W184	I199
L486	K149	Q217	K354	Y422	F185	F185	I199
P487	E150	Q218	R355	F423	W187	W187	S200
S488	L151	S219	L355	A424	Y188	Y188	T201
V489	L152	R220	T356	G425	A256	A256	T202
P490	L152	I221	T426	T426	A257	A257	T203
G491	L155	R222	E427	E427	K258	K258	G204
L495	G156	D223	T428	T428	Y259	Y259	G205
F496	W157	D227	A429	A429	V260	V260	Q206
GLY	T158	E232	T430	T430	I261	I261	E207
LEU	E159	R233	H431	H431	S262	S262	
THR	S160	R234	S432	S432	A263	A263	
THR	A161	P235	S433	S433	I264	I264	
THR	K162	V235	G434	G434	P265	P265	
ILE		F236			P266	P266	
PHE	L167	I237	E437	E437	T267	T267	
SER	F168	V237	G438	G438	L268	L268	
ALA	V169	I238	A439	A439	T201	T201	
THR	N170	D239	V440	V440	G269	G269	
ALA	L171	Q240	E441	E441	M270	M270	
LEU	C172	T241	A442	A442	K271	K271	
GLY	W173	R242	G443	G443	M275	M275	
PHE	T174	E243	S374	S374	P276	P276	
LEU	A175	M244	L375	L375			
LEU		V245	E376	E376			
ALA	H178		A377	A377			
HIS	E179		L378	L378			
LYS	W180						
ARG	S181		V381	V381			
GLY	A182		H382	H382			
LEU	L183						
LEU	W184		N387	N387			
VAL	F185		W388	W388			
ARG	L186		C389	C389			
VAL			E390	E390			
			E391	E391			
			P457	P457			
			P458	P458			
			E459	E459			
			D460	D460			
			E461	E461			
			I462	I462			
			W463	W463			
			Q464	Q464			
			S465	S465			
			E466	E466			
			P467	P467			
			E468	E468			
			S469	S469			
			V470	V470			
			W471	W471			
			D472	D472			
			P473	P473			
			I477	I477			
			F413	F413			
			L414	L414			

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.80 Å   224.30 Å   87.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 3.00 14.90 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.3 (40.00-3.00) 94.5 (14.90-3.08)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.06 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.229 ,   0.271 0.256 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	64.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24034 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NYP, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.71	0/4055	1.17	20/5504 (0.4%)
1	B	0.79	1/4029 (0.0%)	1.21	27/5468 (0.5%)
All	All	0.75	1/8084 (0.0%)	1.19	47/10972 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	TRP	CB-CG	-5.13	1.41	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ASP	CB-CG-OD2	10.68	127.92	118.30
1	B	310	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	54	VAL	CB-CA-C	-7.89	96.41	111.40
1	A	419	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	471	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	330	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	471	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	144	ASP	CB-CG-OD2	7.02	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	375	LEU	CA-CB-CG	-6.79	99.69	115.30
1	B	37	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	223	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	471	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	A	132	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	144	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	64	THR	N-CA-C	6.35	128.13	111.00
1	B	54	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	397	CYS	N-CA-C	6.14	127.58	111.00
1	A	114	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	398	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	404	PRO	C-N-CA	-5.99	109.71	122.30
1	A	235	VAL	CB-CA-C	-5.95	100.09	111.40
1	B	114	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	123	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	173	VAL	CB-CA-C	-5.77	100.44	111.40
1	B	398	TYR	CB-CG-CD1	5.64	124.38	121.00
1	B	227	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	98	PRO	N-CD-CG	-5.62	94.77	103.20
1	A	56	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	A	406	ILE	N-CA-C	5.58	126.06	111.00
1	B	330	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	28	LEU	CA-CB-CG	-5.56	102.51	115.30
1	B	329	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	55	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	397	CYS	N-CA-C	5.34	125.43	111.00
1	A	286	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	460	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	295	ILE	CB-CA-C	-5.25	101.10	111.60
1	B	407	LEU	CA-CB-CG	-5.23	103.27	115.30
1	B	38	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	25	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	37	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	498	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	254	MET	CG-SD-CE	5.11	108.38	100.20
1	A	153	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	311	TYR	CB-CA-C	-5.07	100.26	110.40
1	B	64	THR	N-CA-C	5.03	124.59	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	CYS	Peptide
1	A	405	GLY	Peptide
1	B	397	CYS	Peptide
1	B	405	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3958	0	3959	533	0
1	B	3932	0	3931	435	0
2	A	53	0	29	7	0
2	B	53	0	29	3	0
3	A	12	0	16	12	0
3	B	12	0	16	8	0
All	All	8020	0	7980	945	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:CG2	1:B:208:ARG:HD3	1.66	1.25
1:A:79:THR:CG2	1:A:208:ARG:HD3	1.70	1.20
1:B:175:ALA:HB1	1:B:179:GLU:OE1	1.40	1.19
1:A:82:VAL:HG23	1:A:207:GLU:O	1.43	1.19
1:A:22:LEU:O	1:A:22:LEU:HD12	1.37	1.18
1:A:65:GLN:HB3	1:A:437:GLU:HG3	1.24	1.15
1:B:22:LEU:O	1:B:22:LEU:HD12	1.42	1.15
1:B:82:VAL:HG23	1:B:207:GLU:O	1.45	1.15
1:B:480:THR:HB	1:B:483:GLU:HB2	1.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HG12	1:B:174:THR:N	1.57	1.12
1:B:88:LEU:N	1:B:88:LEU:HD23	1.49	1.12
1:A:304:PRO:HB2	1:A:307:ARG:HD2	1.28	1.12
1:A:51:VAL:HG11	1:A:54:VAL:HG22	1.32	1.12
1:B:64:THR:HG22	1:B:432:TRP:HE1	1.03	1.10
1:A:480:THR:HB	1:A:483:GLU:HB2	1.33	1.10
1:A:79:THR:HG21	1:A:208:ARG:HD3	1.31	1.09
1:A:236:ILE:HD11	1:A:250:LEU:HD12	1.32	1.09
1:B:79:THR:HG21	1:B:208:ARG:HD3	1.29	1.08
1:A:171:LEU:HD13	3:A:601:NYP:H3	1.35	1.08
1:B:125:MET:HE2	1:B:186:LEU:HD11	1.10	1.06
1:A:175:ALA:HB1	1:A:179:GLU:OE1	1.56	1.05
1:A:236:ILE:HD13	1:B:236:ILE:HD13	1.33	1.05
1:A:88:LEU:N	1:A:88:LEU:HD23	1.67	1.04
1:B:323:PRO:HD2	1:B:367:LEU:HD22	1.40	1.04
1:B:264:ILE:CG2	1:B:268:LEU:HB2	1.89	1.03
1:A:456:LYS:O	1:A:457:ILE:HG13	1.56	1.02
1:B:125:MET:HE2	1:B:186:LEU:CD1	1.87	1.02
1:A:304:PRO:HB2	1:A:307:ARG:CD	1.90	1.00
1:B:236:ILE:HD11	1:B:250:LEU:HD12	1.40	1.00
1:A:174:THR:CG2	1:A:293:SER:H	1.75	0.99
1:A:327:THR:O	1:A:328:LEU:HD23	1.63	0.99
1:A:233:ARG:NH1	1:A:253:GLU:OE2	1.96	0.99
1:B:249:THR:HG22	1:B:251:ASN:H	1.22	0.99
1:B:65:GLN:HB3	1:B:437:GLU:HG3	1.41	0.98
1:A:64:THR:HG22	1:A:432:TRP:HE1	1.25	0.98
1:B:249:THR:CG2	1:B:251:ASN:HB2	1.92	0.98
1:A:117:ASN:ND2	1:A:488:SER:HB3	1.80	0.97
1:B:10:VAL:HG22	1:B:235:VAL:HG21	1.45	0.96
1:A:174:THR:O	1:A:174:THR:CG2	2.13	0.96
1:A:67:ARG:N	1:A:437:GLU:OE2	1.98	0.96
1:B:173:VAL:CG1	1:B:174:THR:N	2.29	0.96
1:B:264:ILE:HG23	1:B:268:LEU:HB2	1.45	0.96
1:B:456:LYS:O	1:B:457:ILE:HG13	1.65	0.95
1:B:22:LEU:HD12	1:B:22:LEU:C	1.79	0.95
1:B:79:THR:HG21	1:B:208:ARG:CD	1.97	0.95
1:A:117:ASN:HD22	1:A:488:SER:HB3	1.29	0.95
1:A:264:ILE:HG23	1:A:268:LEU:HB2	1.48	0.94
1:A:201:THR:HG22	1:A:202:THR:N	1.80	0.94
1:A:87:ARG:C	1:A:88:LEU:HD23	1.88	0.93
1:B:264:ILE:HG22	1:B:265:PRO:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:O	1:B:420:ARG:NH1	2.01	0.93
1:B:125:MET:CE	1:B:186:LEU:HD11	1.99	0.92
1:A:270:MET:HG2	1:A:286:ILE:CG2	1.98	0.92
1:B:64:THR:HG22	1:B:432:TRP:NE1	1.85	0.92
1:B:171:LEU:HD13	3:B:601:NYP:H3	1.50	0.92
1:B:79:THR:CG2	1:B:208:ARG:CD	2.49	0.91
1:A:174:THR:CG2	1:A:293:SER:N	2.34	0.91
1:B:67:ARG:N	1:B:437:GLU:OE2	2.03	0.91
1:B:304:PRO:HB2	1:B:307:ARG:HD2	1.52	0.91
1:A:125:MET:CE	1:A:186:LEU:HD11	2.01	0.91
1:A:22:LEU:C	1:A:22:LEU:HD12	1.81	0.91
1:A:258:LYS:O	1:A:259:TYR:CG	2.23	0.91
1:B:88:LEU:N	1:B:88:LEU:CD2	2.27	0.90
1:A:125:MET:HE2	1:A:186:LEU:HD11	1.50	0.90
1:B:173:VAL:HG12	1:B:174:THR:H	1.32	0.90
1:B:448:ARG:NH1	1:B:464:GLN:HB2	1.87	0.90
1:B:171:LEU:O	1:B:171:LEU:HD22	1.72	0.89
1:A:71:LEU:O	1:A:75:LEU:HD12	1.71	0.89
1:A:448:ARG:NH1	1:A:464:GLN:HB2	1.88	0.89
1:B:49:GLN:HG3	1:B:50:LYS:N	1.87	0.88
1:B:174:THR:CG2	1:B:293:SER:H	1.87	0.88
1:B:51:VAL:HG11	1:B:54:VAL:HG22	1.53	0.88
1:B:249:THR:HG22	1:B:251:ASN:HB2	1.52	0.87
1:A:65:GLN:CB	1:A:437:GLU:HG3	2.04	0.87
1:B:70:ARG:NH2	1:B:444:GLU:OE2	2.07	0.87
1:A:323:PRO:HD2	1:A:367:LEU:HD22	1.56	0.87
1:A:315:MET:H	1:A:327:THR:HG22	1.40	0.87
1:B:201:THR:HG22	1:B:202:THR:N	1.87	0.87
1:A:174:THR:HG21	1:A:293:SER:N	1.90	0.87
1:A:171:LEU:HD13	3:A:601:NYP:C3	2.04	0.87
1:A:171:LEU:CD1	3:A:601:NYP:H3	2.04	0.86
1:A:249:THR:HG22	1:A:251:ASN:H	1.40	0.86
1:A:49:GLN:HG3	1:A:50:LYS:N	1.89	0.86
1:A:286:ILE:HG22	1:A:286:ILE:O	1.74	0.86
1:B:71:LEU:O	1:B:75:LEU:HD12	1.76	0.85
1:B:87:ARG:C	1:B:88:LEU:HD23	1.96	0.85
1:A:79:THR:HG21	1:A:208:ARG:CD	2.06	0.85
1:A:79:THR:HG23	1:A:208:ARG:HD3	1.57	0.85
1:B:216:GLN:HA	1:B:219:GLU:HG3	1.56	0.85
1:A:191:GLN:HE22	1:A:433:SER:N	1.75	0.85
1:B:270:MET:HG2	1:B:286:ILE:CG2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:O	1:B:259:TYR:CG	2.30	0.84
1:B:471:ASP:OD1	1:B:471:ASP:N	2.01	0.84
1:A:174:THR:O	1:A:174:THR:HG22	1.78	0.84
1:B:79:THR:HG23	1:B:208:ARG:HD3	1.60	0.84
1:B:268:LEU:O	1:B:271:LYS:HB2	1.78	0.84
1:A:471:ASP:N	1:A:471:ASP:OD1	2.06	0.83
1:A:268:LEU:O	1:A:271:LYS:HB2	1.79	0.83
1:B:425:GLY:O	1:B:428:THR:HB	1.79	0.83
1:B:408:THR:HG22	1:B:409:GLN:HG2	1.61	0.82
1:A:147:THR:HG22	1:A:150:GLU:H	1.45	0.82
1:A:304:PRO:CB	1:A:307:ARG:HD2	2.10	0.82
1:B:270:MET:HG2	1:B:286:ILE:HG22	1.62	0.82
1:A:480:THR:O	1:A:481:PHE:C	2.16	0.82
1:A:488:SER:HB2	1:A:490:PRO:HD2	1.61	0.82
1:A:327:THR:C	1:A:328:LEU:HD23	2.00	0.82
1:B:315:MET:CE	1:B:327:THR:HG21	2.09	0.81
1:A:243:GLU:O	1:A:420:ARG:NH1	2.13	0.81
1:B:240:GLN:OE1	1:B:419:ASP:HB3	1.79	0.81
1:B:144:ASP:OD2	1:B:408:THR:HB	1.80	0.81
1:A:41:GLY:C	1:A:43:THR:H	1.85	0.80
1:A:88:LEU:CD2	1:A:88:LEU:N	2.45	0.80
1:B:174:THR:O	1:B:174:THR:CG2	2.29	0.80
1:B:173:VAL:CG1	1:B:174:THR:H	1.92	0.79
1:A:264:ILE:CG2	1:A:268:LEU:HB2	2.12	0.79
1:B:327:THR:O	1:B:328:LEU:HD23	1.82	0.79
1:B:289:VAL:O	1:B:289:VAL:HG23	1.79	0.79
1:A:64:THR:HG22	1:A:432:TRP:NE1	1.98	0.79
1:B:65:GLN:CB	1:B:437:GLU:HG3	2.12	0.79
1:A:41:GLY:N	1:A:43:THR:HG22	1.98	0.78
1:A:448:ARG:HD2	1:A:461:GLU:O	1.83	0.78
1:A:258:LYS:O	1:A:259:TYR:CD1	2.36	0.78
1:B:86:GLU:OE2	1:B:86:GLU:N	2.16	0.78
1:A:79:THR:CG2	1:A:208:ARG:CD	2.60	0.78
1:A:251:ASN:O	1:A:252:HIS:HB2	1.83	0.78
1:A:129:ILE:O	1:A:190:LYS:HE2	1.83	0.77
1:B:249:THR:HG21	1:B:251:ASN:HB2	1.66	0.77
1:B:251:ASN:O	1:B:252:HIS:HB2	1.84	0.77
1:A:173:VAL:HG12	1:A:174:THR:H	1.48	0.77
1:A:174:THR:HG22	1:A:293:SER:H	1.48	0.77
1:A:209:LYS:NZ	1:A:330:ASP:OD1	2.17	0.77
1:A:30:VAL:CG1	1:A:31:VAL:N	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:CD2	1:B:171:LEU:O	2.33	0.76
1:B:47:ARG:NH2	1:B:219:GLU:OE1	2.17	0.76
1:A:265:PRO:HD2	1:A:268:LEU:HD12	1.68	0.76
1:B:174:THR:O	1:B:174:THR:HG23	1.84	0.76
1:B:125:MET:CE	1:B:186:LEU:CD1	2.62	0.76
1:A:79:THR:HG21	1:A:208:ARG:HH11	1.50	0.76
1:A:64:THR:CG2	1:A:432:TRP:HE1	1.98	0.76
1:B:92:VAL:HG22	1:B:318:ASP:CB	2.15	0.76
1:A:86:GLU:N	1:A:86:GLU:OE2	2.18	0.75
1:A:65:GLN:HB3	1:A:437:GLU:CG	2.13	0.75
1:B:174:THR:CG2	1:B:293:SER:N	2.49	0.75
1:B:171:LEU:CD1	3:B:601:NYP:H3	2.15	0.75
1:A:10:VAL:HG22	1:A:235:VAL:HG21	1.69	0.75
1:B:117:ASN:ND2	1:B:488:SER:HB3	2.01	0.74
1:B:174:THR:HG21	1:B:293:SER:N	2.02	0.74
1:B:174:THR:HG22	1:B:293:SER:H	1.51	0.74
1:A:236:ILE:CD1	1:A:250:LEU:HD12	2.13	0.74
1:B:171:LEU:HD13	3:B:601:NYP:C3	2.17	0.74
1:B:315:MET:H	1:B:327:THR:HG22	1.52	0.74
1:A:288:ARG:NH2	1:B:291:LEU:O	2.20	0.74
1:A:293:SER:HB3	1:A:389:CYS:SG	2.28	0.74
1:A:286:ILE:O	1:A:286:ILE:CG2	2.36	0.74
1:B:253:GLU:OE1	1:B:255:TYR:OH	2.02	0.74
1:B:117:ASN:HD22	1:B:488:SER:CB	2.00	0.73
1:B:64:THR:CG2	1:B:432:TRP:HE1	1.93	0.73
1:A:428:THR:HG23	1:A:445:ARG:HH12	1.53	0.73
1:A:120:ARG:NH2	1:A:486:LEU:O	2.22	0.73
1:B:7:VAL:HG22	1:B:259:TYR:HB2	1.69	0.73
1:A:171:LEU:CD1	3:A:601:NYP:H2	2.18	0.73
1:A:173:VAL:HG12	1:A:174:THR:N	2.02	0.72
1:B:480:THR:O	1:B:481:PHE:C	2.28	0.72
1:A:282:ARG:NH2	1:A:423:PHE:CE2	2.57	0.72
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.87	0.72
1:B:54:VAL:CG1	1:B:300:TYR:OH	2.35	0.72
1:A:287:THR:HG23	1:A:287:THR:O	1.88	0.72
1:B:209:LYS:NZ	1:B:330:ASP:OD1	2.22	0.72
1:B:22:LEU:CD1	1:B:22:LEU:C	2.56	0.72
1:B:188:TYR:O	1:B:191:GLN:HG3	1.89	0.72
1:A:71:LEU:O	1:A:75:LEU:CD1	2.37	0.72
1:A:249:THR:CG2	1:A:251:ASN:HB2	2.19	0.71
1:B:78:GLU:O	1:B:211:VAL:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG22	1:A:251:ASN:HB2	1.72	0.71
1:A:264:ILE:HG23	1:A:268:LEU:CB	2.19	0.71
1:A:300:TYR:CD2	1:A:339:ALA:HB2	2.25	0.71
1:A:37:ASP:O	1:A:231:LEU:HD13	1.90	0.71
1:A:285:MET:C	1:A:287:THR:H	1.92	0.71
1:B:41:GLY:C	1:B:43:THR:H	1.94	0.71
1:B:111:THR:HG23	1:B:158:THR:HG21	1.72	0.71
1:A:43:THR:O	1:A:43:THR:HG22	1.90	0.71
1:A:408:THR:HG22	1:A:409:GLN:HG2	1.71	0.71
2:A:600:FAD:O2A	2:A:600:FAD:O5'	2.07	0.70
2:B:600:FAD:O5'	2:B:600:FAD:O2A	2.07	0.70
1:A:43:THR:CG2	1:A:43:THR:O	2.39	0.70
1:A:240:GLN:OE1	1:A:419:ASP:HB3	1.90	0.70
1:A:174:THR:HG23	1:A:174:THR:O	1.92	0.70
1:A:425:GLY:O	1:A:428:THR:HB	1.91	0.70
1:A:428:THR:CG2	1:A:445:ARG:HH12	2.05	0.70
1:A:28:LEU:HD13	1:A:454:MET:HE1	1.73	0.70
1:B:88:LEU:H	1:B:88:LEU:HD23	1.54	0.70
1:B:10:VAL:CG2	1:B:235:VAL:HG21	2.22	0.70
1:A:117:ASN:HD22	1:A:488:SER:CB	2.03	0.70
1:B:239:ASP:OD1	1:B:241:THR:HB	1.92	0.70
1:B:249:THR:HG22	1:B:251:ASN:N	2.02	0.69
1:B:28:LEU:HD13	1:B:454:MET:HE1	1.74	0.69
1:B:117:ASN:HD22	1:B:488:SER:HB3	1.56	0.69
1:A:314:THR:HA	1:A:327:THR:O	1.92	0.69
1:A:291:LEU:HD23	1:A:400:THR:HA	1.74	0.69
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.27	0.69
1:B:198:ILE:HG22	1:B:199:ILE:HG13	1.73	0.69
1:A:275:ASN:HA	1:A:276:PRO:C	2.13	0.69
1:B:293:SER:HB3	1:B:389:CYS:SG	2.32	0.69
1:B:265:PRO:HD2	1:B:268:LEU:HD12	1.74	0.69
1:B:63:PRO:HG2	1:B:204:GLY:HA2	1.73	0.69
1:B:275:ASN:HA	1:B:276:PRO:C	2.13	0.69
1:B:12:GLY:HA3	1:B:34:GLU:OE1	1.93	0.68
1:B:315:MET:HE2	1:B:327:THR:HG21	1.74	0.68
1:B:79:THR:HG21	1:B:208:ARG:HH11	1.58	0.68
1:B:387:ASN:O	1:B:390:GLU:HG2	1.93	0.68
1:B:300:TYR:CD2	1:B:339:ALA:HB2	2.29	0.68
1:B:37:ASP:OD1	1:B:37:ASP:N	2.16	0.68
1:A:143:TRP:HA	1:A:146:MET:CE	2.24	0.68
1:A:488:SER:CB	1:A:490:PRO:HD2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:HG22	1:A:400:THR:H	1.60	0.67
1:A:22:LEU:C	1:A:22:LEU:CD1	2.59	0.67
1:A:54:VAL:HG13	1:A:300:TYR:OH	1.95	0.67
1:B:240:GLN:NE2	1:B:421:ILE:HG13	2.10	0.67
1:A:280:MET:HG3	1:B:389:CYS:HB3	1.76	0.67
1:B:236:ILE:HG22	1:B:237:TYR:HB2	1.77	0.67
1:A:364:LEU:O	1:A:367:LEU:HB3	1.94	0.67
1:A:34:GLU:OE1	2:A:600:FAD:O3B	2.12	0.67
1:A:451:LEU:HB3	1:A:457:ILE:HD12	1.77	0.67
1:B:320:GLU:OE2	1:B:347:HIS:CE1	2.46	0.67
1:B:431:HIS:O	1:B:432:TRP:C	2.29	0.67
1:A:82:VAL:CG2	1:A:207:GLU:O	2.33	0.67
1:B:92:VAL:HG22	1:B:318:ASP:HB2	1.77	0.67
1:A:37:ASP:OD1	1:A:37:ASP:N	2.28	0.67
1:A:119:TRP:CE3	1:A:195:THR:HG21	2.29	0.67
1:A:315:MET:CE	1:A:327:THR:HG21	2.24	0.67
1:B:428:THR:CG2	1:B:445:ARG:HH12	2.06	0.67
1:A:448:ARG:NH1	1:A:462:ILE:O	2.28	0.66
1:B:220:ARG:HA	1:B:223:ASP:OD2	1.95	0.66
1:A:86:GLU:HG2	1:A:312:CYS:HB3	1.77	0.66
1:A:431:HIS:CD2	1:A:432:TRP:CD1	2.84	0.66
1:B:456:LYS:O	1:B:457:ILE:CG1	2.40	0.66
1:B:54:VAL:HG13	1:B:300:TYR:OH	1.95	0.66
1:B:291:LEU:HD23	1:B:400:THR:HA	1.77	0.66
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.31	0.66
1:B:315:MET:HE3	1:B:327:THR:HG21	1.76	0.66
1:A:51:VAL:HG11	1:A:54:VAL:CG2	2.19	0.66
1:A:264:ILE:HG22	1:A:265:PRO:O	1.96	0.65
1:A:24:HIS:C	1:A:26:SER:H	1.99	0.65
1:B:264:ILE:HG23	1:B:268:LEU:CB	2.23	0.65
1:A:304:PRO:CB	1:A:307:ARG:CD	2.71	0.65
1:A:343:PHE:HB3	1:A:345:LEU:HD21	1.78	0.65
1:A:51:VAL:CG1	1:A:54:VAL:HG22	2.19	0.65
1:A:275:ASN:OD1	1:A:276:PRO:HA	1.97	0.65
1:A:399:THR:CG2	1:A:400:THR:H	2.08	0.65
1:A:270:MET:HG2	1:A:286:ILE:HG22	1.78	0.65
1:B:30:VAL:CG1	1:B:31:VAL:N	2.59	0.65
1:B:286:ILE:HG22	1:B:286:ILE:O	1.96	0.65
1:A:4:LYS:HB2	1:A:256:GLU:HG3	1.78	0.65
1:B:428:THR:HG23	1:B:445:ARG:HH12	1.61	0.65
1:B:43:THR:HG22	1:B:43:THR:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG22	1:A:292:GLY:CA	2.27	0.65
1:A:236:ILE:HG22	1:A:237:TYR:HB2	1.79	0.65
1:B:65:GLN:HB3	1:B:437:GLU:CG	2.22	0.64
1:A:191:GLN:HE22	1:A:433:SER:CA	2.09	0.64
1:A:168:PHE:CG	1:A:168:PHE:O	2.50	0.64
1:A:491:GLY:O	1:A:494:ARG:HG2	1.96	0.64
1:B:134:PRO:HG2	1:B:407:LEU:HD21	1.78	0.64
1:A:47:ARG:NH2	1:A:219:GLU:OE1	2.28	0.64
1:B:264:ILE:CG2	1:B:268:LEU:CB	2.73	0.64
1:B:304:PRO:CB	1:B:307:ARG:HD2	2.27	0.64
1:B:387:ASN:OD1	1:B:389:CYS:HB2	1.97	0.64
1:A:456:LYS:O	1:A:457:ILE:CG1	2.39	0.64
1:B:448:ARG:NH1	1:B:462:ILE:O	2.30	0.64
1:A:216:GLN:HA	1:A:219:GLU:HG3	1.80	0.64
1:A:174:THR:CG2	1:A:292:GLY:HA3	2.28	0.64
1:B:323:PRO:HD2	1:B:367:LEU:CD2	2.25	0.64
1:A:144:ASP:OD2	1:A:408:THR:HB	1.96	0.64
1:B:233:ARG:NH1	1:B:253:GLU:OE2	2.30	0.64
1:A:287:THR:HG22	1:A:288:ARG:HG3	1.79	0.64
1:A:236:ILE:HG22	1:A:237:TYR:CB	2.28	0.64
1:A:86:GLU:HB2	1:A:312:CYS:N	2.13	0.64
1:A:456:LYS:C	1:A:457:ILE:HG13	2.18	0.64
1:A:248:GLU:OE2	1:B:252:HIS:NE2	2.30	0.64
1:A:28:LEU:CD1	1:A:454:MET:CE	2.76	0.63
1:A:267:THR:HG22	1:B:270:MET:CE	2.29	0.63
1:A:426:THR:C	1:A:428:THR:H	2.01	0.63
1:B:406:ILE:O	1:B:407:LEU:C	2.35	0.63
1:A:89:ILE:CG2	1:A:96:SER:HB3	2.29	0.63
1:A:315:MET:N	1:A:327:THR:HG22	2.12	0.63
1:A:125:MET:CE	1:A:186:LEU:CD1	2.76	0.63
1:B:216:GLN:CA	1:B:219:GLU:HG3	2.27	0.63
1:A:381:VAL:O	1:A:381:VAL:HG13	1.99	0.63
1:A:171:LEU:HD13	3:A:601:NYP:C2	2.29	0.63
1:B:448:ARG:HD2	1:B:461:GLU:O	1.98	0.63
1:A:109:PRO:C	1:A:111:THR:H	2.02	0.63
1:B:147:THR:HG22	1:B:150:GLU:H	1.64	0.63
1:A:446:ALA:O	1:A:449:GLU:HB2	1.99	0.62
1:B:36:ARG:NH1	1:B:391:GLU:OE1	2.32	0.62
1:A:270:MET:HG2	1:A:286:ILE:HG21	1.81	0.62
1:A:12:GLY:HA3	1:A:34:GLU:OE1	1.99	0.62
1:A:236:ILE:CD1	1:B:236:ILE:HD13	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG12	1:A:31:VAL:N	2.14	0.62
1:A:289:VAL:HG23	1:A:289:VAL:O	1.99	0.62
1:A:41:GLY:H	1:A:43:THR:HG22	1.63	0.62
1:A:171:LEU:HD13	3:A:601:NYP:H2	1.82	0.62
1:A:258:LYS:O	1:A:259:TYR:CD2	2.52	0.62
1:B:191:GLN:HE22	1:B:433:SER:N	1.96	0.62
1:A:489:VAL:N	1:A:490:PRO:CD	2.62	0.62
1:B:428:THR:O	1:B:428:THR:HG23	2.00	0.62
1:B:41:GLY:C	1:B:43:THR:N	2.51	0.62
1:B:249:THR:HG22	1:B:251:ASN:CB	2.28	0.62
1:A:126:GLY:C	1:A:128:GLU:H	2.02	0.62
1:A:240:GLN:NE2	1:A:418:VAL:O	2.23	0.62
1:A:285:MET:C	1:A:287:THR:N	2.53	0.61
1:A:252:HIS:CE1	1:B:248:GLU:OE2	2.52	0.61
1:B:92:VAL:HG22	1:B:318:ASP:HB3	1.82	0.61
1:B:343:PHE:HB3	1:B:345:LEU:HD21	1.82	0.61
1:A:178:HIS:CE1	1:B:145:ASN:OD1	2.53	0.61
1:A:287:THR:HG23	1:B:290:PRO:HB3	1.83	0.61
1:B:400:THR:OG1	1:B:427:GLU:OE1	2.10	0.61
1:A:233:ARG:NH1	1:A:253:GLU:CD	2.53	0.61
1:B:320:GLU:OE2	1:B:347:HIS:NE2	2.33	0.61
1:B:182:ALA:O	1:B:183:LEU:C	2.38	0.61
1:A:46:LEU:HB3	1:A:54:VAL:HG23	1.82	0.61
1:B:337:TYR:O	1:B:338:ALA:C	2.35	0.61
1:A:191:GLN:NE2	1:A:433:SER:N	2.48	0.61
1:B:54:VAL:HG11	1:B:300:TYR:OH	2.00	0.61
1:B:34:GLU:OE1	2:B:600:FAD:O3B	2.19	0.61
1:B:70:ARG:HH22	1:B:444:GLU:CD	2.04	0.60
1:A:151:LEU:O	1:A:155:LEU:HB2	2.01	0.60
1:A:168:PHE:CE1	1:A:199:ILE:HD11	2.36	0.60
1:A:28:LEU:HD11	1:A:454:MET:CE	2.32	0.60
1:B:258:LYS:O	1:B:259:TYR:CD2	2.54	0.60
1:B:446:ALA:O	1:B:449:GLU:N	2.33	0.60
1:A:55:ASP:OD2	1:A:59:SER:OG	2.18	0.60
1:A:41:GLY:C	1:A:43:THR:N	2.51	0.60
1:A:79:THR:HG22	1:A:80:TYR:N	2.15	0.60
1:A:426:THR:HG23	1:A:427:GLU:N	2.16	0.60
1:B:126:GLY:C	1:B:128:GLU:H	2.05	0.60
1:A:236:ILE:O	1:A:236:ILE:CG2	2.48	0.60
1:A:209:LYS:CE	1:A:330:ASP:OD1	2.50	0.59
1:A:173:VAL:CG1	1:A:174:THR:H	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD11	3:A:601:NYP:H2	1.84	0.59
1:A:5:CYS:SG	1:A:6:ASP:N	2.75	0.59
1:A:291:LEU:HD12	1:A:395:GLY:C	2.23	0.59
1:A:75:LEU:N	1:A:75:LEU:HD12	2.17	0.59
1:A:28:LEU:HD11	1:A:454:MET:HE3	1.83	0.59
1:B:71:LEU:O	1:B:75:LEU:CD1	2.49	0.59
1:B:426:THR:C	1:B:428:THR:H	2.05	0.59
1:B:6:ASP:HB2	1:B:29:ASN:HB2	1.83	0.59
1:A:68:ILE:HD12	1:A:436:MET:HB3	1.85	0.59
1:B:313:GLY:O	1:B:327:THR:CG2	2.50	0.59
1:B:63:PRO:HG2	1:B:204:GLY:CA	2.32	0.59
1:B:67:ARG:NH2	1:B:466:GLU:HG2	2.17	0.59
1:A:267:THR:HG22	1:B:270:MET:HE1	1.84	0.59
1:A:378:LEU:HD23	1:A:378:LEU:N	2.16	0.59
1:A:79:THR:CG2	1:A:80:TYR:N	2.66	0.58
1:B:307:ARG:O	1:B:310:ASP:N	2.32	0.58
1:A:28:LEU:CD1	1:A:454:MET:HE1	2.33	0.58
1:B:68:ILE:HG22	1:B:437:GLU:HG2	1.85	0.58
1:B:456:LYS:C	1:B:457:ILE:HG13	2.22	0.58
1:A:172:CYS:SG	3:A:601:NYP:H5	2.44	0.58
1:A:252:HIS:ND1	1:B:252:HIS:CE1	2.72	0.58
1:A:6:ASP:HB2	1:A:29:ASN:O	2.03	0.58
1:B:21:LYS:O	1:B:22:LEU:C	2.39	0.58
1:A:41:GLY:H	1:A:43:THR:CG2	2.14	0.58
1:B:79:THR:HG23	1:B:208:ARG:CD	2.25	0.58
1:B:206:GLN:NE2	3:B:601:NYP:H8N1	2.19	0.58
1:A:7:VAL:HG22	1:A:259:TYR:HB2	1.84	0.58
1:A:30:VAL:HG13	1:A:31:VAL:N	2.18	0.58
1:B:233:ARG:CD	1:B:251:ASN:HD22	2.17	0.58
1:A:30:VAL:O	1:A:31:VAL:HG23	2.04	0.57
1:A:413:VAL:HG12	1:A:413:VAL:O	2.04	0.57
1:B:489:VAL:N	1:B:490:PRO:CD	2.67	0.57
1:A:285:MET:O	1:A:287:THR:N	2.38	0.57
1:B:346:ALA:O	1:B:349:ALA:N	2.36	0.57
1:B:285:MET:C	1:B:287:THR:H	2.08	0.57
1:B:291:LEU:HD22	1:B:399:THR:C	2.24	0.57
1:A:482:LEU:O	1:A:486:LEU:HG	2.04	0.57
1:A:119:TRP:HE3	1:A:195:THR:HG21	1.67	0.57
1:A:134:PRO:HD2	1:A:135:TRP:CE3	2.40	0.57
1:A:215:GLY:O	1:A:219:GLU:HG2	2.04	0.57
1:B:157:TRP:CZ2	1:B:490:PRO:HG3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:C	1:B:171:LEU:HD22	2.25	0.57
1:B:85:VAL:HB	1:B:86:GLU:OE2	2.04	0.57
1:A:236:ILE:HD13	1:B:236:ILE:CD1	2.23	0.56
1:A:24:HIS:C	1:A:26:SER:N	2.54	0.56
1:A:315:MET:HE3	1:A:327:THR:HG21	1.86	0.56
1:A:438:GLY:O	1:A:439:ALA:C	2.39	0.56
1:B:249:THR:CG2	1:B:251:ASN:CB	2.78	0.56
1:B:285:MET:CE	1:B:414:LEU:HD23	2.35	0.56
1:A:126:GLY:O	1:A:190:LYS:HD3	2.06	0.56
1:A:23:LEU:O	1:A:26:SER:HB3	2.05	0.56
1:A:92:VAL:O	1:A:93:LYS:HB2	2.05	0.56
1:A:10:VAL:CG2	1:A:235:VAL:HG21	2.33	0.56
1:A:126:GLY:C	1:A:128:GLU:N	2.58	0.56
1:B:290:PRO:O	1:B:400:THR:HA	2.06	0.56
1:A:291:LEU:HD22	1:A:399:THR:O	2.05	0.56
1:A:38:ARG:NH2	1:A:41:GLY:O	2.37	0.56
1:B:48:ASN:OD1	1:B:48:ASN:C	2.44	0.56
1:B:236:ILE:HG22	1:B:237:TYR:CB	2.36	0.56
1:B:287:THR:HG23	1:B:287:THR:O	2.05	0.56
1:B:54:VAL:HG13	1:B:300:TYR:HH	1.70	0.56
1:B:38:ARG:NH2	1:B:41:GLY:O	2.39	0.56
1:B:428:THR:O	1:B:428:THR:CG2	2.52	0.56
1:A:285:MET:HE1	1:A:414:LEU:HD23	1.88	0.56
1:A:291:LEU:HD22	1:A:399:THR:C	2.26	0.56
1:A:40:GLY:CA	1:A:43:THR:HG22	2.36	0.55
1:B:430:THR:HB	1:B:441:GLU:OE2	2.06	0.55
1:A:48:ASN:OD1	1:A:48:ASN:C	2.43	0.55
1:B:426:THR:HB	1:B:439:ALA:HB2	1.88	0.55
1:B:24:HIS:C	1:B:26:SER:H	2.09	0.55
1:A:147:THR:HG22	1:A:147:THR:O	2.05	0.55
1:A:119:TRP:CE3	1:A:195:THR:CG2	2.88	0.55
1:A:80:TYR:CE2	1:A:209:LYS:HB2	2.41	0.55
1:A:481:PHE:O	1:A:485:HIS:HD2	1.89	0.55
1:B:82:VAL:CG2	1:B:207:GLU:O	2.36	0.55
1:B:65:GLN:CA	1:B:437:GLU:HG3	2.37	0.55
1:A:290:PRO:HB3	1:B:287:THR:HG23	1.87	0.55
1:A:86:GLU:H	1:A:86:GLU:CD	2.08	0.55
1:B:24:HIS:C	1:B:26:SER:N	2.59	0.55
1:A:174:THR:CG2	1:A:292:GLY:CA	2.84	0.55
1:A:252:HIS:CE1	1:B:252:HIS:ND1	2.75	0.55
1:B:171:LEU:CD2	1:B:171:LEU:C	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:CB	1:B:304:PRO:CD	2.84	0.55
1:A:291:LEU:HD12	1:A:395:GLY:CA	2.37	0.55
1:A:188:TYR:O	1:A:191:GLN:HG3	2.06	0.55
1:B:126:GLY:C	1:B:128:GLU:N	2.60	0.55
1:A:309:LYS:NZ	1:A:373:GLY:O	2.40	0.55
1:A:458:PRO:O	1:A:459:GLU:C	2.46	0.55
1:B:444:GLU:HB3	1:B:448:ARG:HH21	1.71	0.55
1:A:125:MET:HE2	1:A:186:LEU:CD1	2.30	0.55
1:A:114:ASP:O	1:A:115:HIS:C	2.43	0.55
1:B:110:ILE:O	1:B:110:ILE:HG22	2.07	0.55
1:A:78:GLU:O	1:A:211:VAL:HG23	2.07	0.55
1:A:239:ASP:OD1	1:A:241:THR:HB	2.07	0.55
1:A:387:ASN:O	1:A:390:GLU:HG2	2.06	0.54
1:B:92:VAL:CG2	1:B:318:ASP:HB2	2.36	0.54
1:B:41:GLY:N	1:B:43:THR:HG22	2.22	0.54
1:A:320:GLU:C	1:A:322:ALA:H	2.10	0.54
1:A:303:GLU:CB	1:A:304:PRO:CD	2.85	0.54
1:A:173:VAL:CG1	1:A:174:THR:N	2.68	0.54
1:A:295:ILE:HG12	1:A:387:ASN:HB2	1.88	0.54
1:A:406:ILE:O	1:A:407:LEU:C	2.45	0.54
1:A:291:LEU:HD12	1:A:395:GLY:HA3	1.89	0.54
1:B:171:LEU:CD1	3:B:601:NYP:H2	2.37	0.54
1:A:301:TYR:O	1:A:338:ALA:HB3	2.07	0.54
1:B:392:GLN:HG2	1:B:393:TYR:CE1	2.43	0.54
1:A:431:HIS:O	1:A:432:TRP:C	2.45	0.54
1:B:287:THR:HG22	1:B:288:ARG:HG3	1.89	0.54
1:A:171:LEU:HA	1:A:345:LEU:HD13	1.88	0.54
1:B:332:LYS:HB3	1:B:333:PRO:CD	2.36	0.54
1:A:430:THR:HB	1:A:441:GLU:OE2	2.06	0.54
1:A:365:CYS:O	1:A:366:GLU:C	2.45	0.54
1:B:198:ILE:CG2	1:B:199:ILE:N	2.69	0.54
1:B:258:LYS:O	1:B:259:TYR:CD1	2.61	0.54
1:B:315:MET:N	1:B:327:THR:HG22	2.22	0.54
1:A:16:GLY:O	1:A:19:ALA:N	2.40	0.54
1:A:271:LYS:HD3	1:B:270:MET:O	2.07	0.54
1:B:346:ALA:O	1:B:347:HIS:C	2.45	0.54
1:A:480:THR:O	1:A:482:LEU:N	2.41	0.53
1:B:159:GLU:O	1:B:160:SER:C	2.45	0.53
1:B:232:GLU:C	1:B:234:PRO:HD3	2.29	0.53
1:A:171:LEU:HA	1:A:345:LEU:CD1	2.39	0.53
1:A:315:MET:HE2	1:A:327:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ILE:HG22	1:B:199:ILE:N	2.23	0.53
1:A:92:VAL:HG22	1:A:318:ASP:HB2	1.91	0.53
1:B:120:ARG:NH2	1:B:486:LEU:O	2.38	0.53
1:A:405:GLY:C	1:A:406:ILE:HG13	2.29	0.53
1:B:285:MET:O	1:B:287:THR:N	2.42	0.53
1:A:305:PHE:CE1	1:A:306:TRP:HZ3	2.26	0.53
1:B:87:ARG:C	1:B:88:LEU:CD2	2.71	0.53
1:B:304:PRO:HB2	1:B:307:ARG:CD	2.32	0.53
1:B:388:TRP:O	1:B:389:CYS:C	2.46	0.53
1:A:269:GLY:C	1:A:271:LYS:H	2.11	0.53
1:B:331:THR:OG1	1:B:338:ALA:HA	2.09	0.53
1:A:236:ILE:O	1:A:236:ILE:HG23	2.08	0.53
1:A:269:GLY:C	1:A:271:LYS:N	2.62	0.53
1:B:413:VAL:O	1:B:413:VAL:HG12	2.07	0.53
1:A:62:GLY:O	1:A:63:PRO:C	2.47	0.53
1:A:251:ASN:O	1:A:252:HIS:CB	2.51	0.53
1:B:64:THR:O	1:B:64:THR:HG23	2.08	0.52
1:A:168:PHE:CD1	1:A:168:PHE:O	2.62	0.52
1:B:365:CYS:O	1:B:368:TYR:N	2.43	0.52
1:A:174:THR:HG22	1:A:293:SER:N	2.14	0.52
1:A:167:LEU:HD11	1:A:325:ALA:HB1	1.91	0.52
1:B:40:GLY:CA	1:B:43:THR:HG22	2.39	0.52
1:A:21:LYS:O	1:A:22:LEU:C	2.46	0.52
1:A:297:CYS:C	1:A:298:ILE:HD12	2.30	0.52
1:A:198:ILE:HG22	1:A:199:ILE:HG13	1.90	0.52
1:B:431:HIS:O	1:B:433:SER:N	2.42	0.52
1:B:51:VAL:HG12	1:B:51:VAL:O	2.10	0.52
1:B:41:GLY:H	1:B:43:THR:CG2	2.23	0.52
1:B:368:TYR:O	1:B:372:LEU:HB2	2.09	0.52
1:A:36:ARG:NH1	1:A:391:GLU:OE1	2.43	0.52
1:B:49:GLN:CG	1:B:50:LYS:N	2.67	0.52
1:A:240:GLN:CD	1:A:419:ASP:HB3	2.29	0.52
1:A:426:THR:C	1:A:428:THR:N	2.61	0.52
1:A:64:THR:O	1:A:64:THR:HG23	2.10	0.52
1:B:481:PHE:O	1:B:485:HIS:HD2	1.93	0.52
1:A:337:TYR:O	1:A:338:ALA:C	2.47	0.52
1:B:336:ASN:HB3	1:B:337:TYR:HD1	1.74	0.52
1:A:285:MET:CE	1:A:414:LEU:HA	2.40	0.52
1:A:480:THR:O	1:A:483:GLU:N	2.43	0.52
1:A:275:ASN:OD1	1:A:276:PRO:CA	2.58	0.52
1:A:110:ILE:HG22	1:A:110:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:THR:O	1:B:207:GLU:OE1	2.27	0.52
1:B:30:VAL:HG12	1:B:31:VAL:N	2.25	0.52
1:A:249:THR:HG21	1:A:251:ASN:HB2	1.92	0.51
1:B:458:PRO:O	1:B:459:GLU:C	2.47	0.51
1:A:264:ILE:CG2	1:A:268:LEU:CB	2.84	0.51
1:A:388:TRP:O	1:A:390:GLU:N	2.43	0.51
1:A:236:ILE:HD11	1:A:250:LEU:CD1	2.23	0.51
1:B:249:THR:C	1:B:251:ASN:N	2.63	0.51
1:B:209:LYS:HZ3	1:B:330:ASP:CG	2.13	0.51
1:B:40:GLY:HA3	1:B:43:THR:HG22	1.92	0.51
1:A:337:TYR:N	1:A:337:TYR:CD1	2.77	0.51
1:B:91:HIS:HA	1:B:95:LYS:O	2.11	0.51
1:B:446:ALA:O	1:B:447:ALA:C	2.47	0.51
1:A:320:GLU:OE2	1:A:347:HIS:CE1	2.64	0.51
1:A:293:SER:CB	1:A:389:CYS:SG	2.98	0.51
1:A:285:MET:CE	1:A:414:LEU:HD23	2.41	0.51
1:A:40:GLY:C	1:A:43:THR:HG22	2.31	0.51
1:A:269:GLY:O	1:A:271:LYS:N	2.43	0.51
1:B:51:VAL:CG1	1:B:51:VAL:O	2.59	0.51
1:B:167:LEU:O	1:B:168:PHE:C	2.46	0.51
1:A:134:PRO:HG2	1:A:407:LEU:HD21	1.92	0.51
1:A:313:GLY:O	1:A:327:THR:CG2	2.59	0.51
1:B:285:MET:CE	1:B:414:LEU:HA	2.41	0.51
1:A:246:LEU:HD23	1:A:256:GLU:HB3	1.91	0.51
1:B:189:VAL:HG12	1:B:194:GLY:HA2	1.92	0.51
1:B:17:MET:O	1:B:18:ALA:C	2.48	0.51
1:A:54:VAL:CG1	1:A:300:TYR:OH	2.58	0.51
1:A:291:LEU:O	1:B:288:ARG:NH2	2.44	0.51
1:B:171:LEU:HD13	3:B:601:NYP:C2	2.41	0.51
1:B:6:ASP:HB2	1:B:29:ASN:O	2.11	0.51
1:A:426:THR:HG23	1:A:427:GLU:HG2	1.92	0.51
1:A:459:GLU:O	1:A:462:ILE:HG13	2.10	0.51
1:B:270:MET:CG	1:B:286:ILE:HG22	2.37	0.51
1:B:309:LYS:NZ	1:B:373:GLY:O	2.44	0.51
1:B:285:MET:HE1	1:B:414:LEU:HD23	1.92	0.50
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.93	0.50
1:A:389:CYS:HB3	1:B:280:MET:HG3	1.94	0.50
1:A:327:THR:HA	1:A:341:MET:O	2.10	0.50
1:B:313:GLY:O	1:B:327:THR:HG22	2.11	0.50
1:B:240:GLN:CD	1:B:419:ASP:HB3	2.32	0.50
1:B:282:ARG:NH2	1:B:423:PHE:CE2	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:C	1:A:111:THR:N	2.65	0.50
1:B:117:ASN:ND2	1:B:488:SER:CB	2.67	0.50
1:A:111:THR:HG23	1:A:158:THR:HG21	1.93	0.50
1:B:151:LEU:O	1:B:155:LEU:HB2	2.12	0.50
1:A:365:CYS:O	1:A:368:TYR:N	2.45	0.50
1:B:442:ALA:O	1:B:443:GLY:C	2.50	0.50
1:B:168:PHE:CE1	1:B:172:CYS:SG	3.05	0.50
1:A:216:GLN:O	1:A:217:VAL:C	2.47	0.50
1:A:290:PRO:O	1:A:400:THR:HA	2.11	0.50
1:B:381:VAL:O	1:B:382:HIS:HB2	2.12	0.50
1:A:88:LEU:O	1:A:98:PRO:HA	2.12	0.50
1:A:6:ASP:OD2	1:A:28:LEU:HD22	2.12	0.50
1:A:364:LEU:HB3	1:A:368:TYR:CE1	2.46	0.50
1:A:144:ASP:OD2	1:A:408:THR:CB	2.60	0.50
1:A:134:PRO:HG3	1:A:187:TRP:CD1	2.47	0.49
1:A:266:PRO:O	1:A:267:THR:C	2.51	0.49
1:A:448:ARG:NH1	1:A:464:GLN:CB	2.69	0.49
1:A:336:ASN:HB3	1:A:337:TYR:HD1	1.77	0.49
1:A:79:THR:HG23	1:A:208:ARG:CD	2.35	0.49
1:A:446:ALA:O	1:A:447:ALA:C	2.50	0.49
1:B:282:ARG:O	1:B:285:MET:N	2.45	0.49
1:A:411:GLY:O	1:A:413:VAL:N	2.45	0.49
1:A:291:LEU:HD23	1:A:400:THR:CA	2.43	0.49
1:B:75:LEU:N	1:B:75:LEU:HD12	2.26	0.49
1:B:327:THR:HA	1:B:341:MET:O	2.12	0.49
1:B:167:LEU:HD11	1:B:325:ALA:HB1	1.93	0.49
1:A:198:ILE:HG22	1:A:199:ILE:N	2.28	0.49
1:A:196:THR:O	1:A:197:ARG:C	2.49	0.49
1:A:209:LYS:HZ1	1:A:330:ASP:CG	2.15	0.49
1:B:236:ILE:CD1	1:B:250:LEU:HD12	2.28	0.49
1:A:446:ALA:O	1:A:449:GLU:N	2.43	0.49
1:A:89:ILE:HG23	1:A:96:SER:HB3	1.94	0.49
1:B:171:LEU:HD13	3:B:601:NYP:H2	1.94	0.49
1:A:306:TRP:CZ3	1:A:340:ILE:HD11	2.48	0.49
1:A:68:ILE:HG22	1:A:437:GLU:HG2	1.95	0.49
1:B:134:PRO:HD2	1:B:135:TRP:CZ3	2.48	0.49
1:A:148:MET:O	1:A:152:LEU:HG	2.13	0.49
1:B:426:THR:OG1	1:B:434:GLY:N	2.38	0.49
1:B:405:GLY:C	1:B:406:ILE:HG13	2.33	0.49
1:A:92:VAL:HG22	1:A:318:ASP:CB	2.43	0.49
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	1:A:466:GLU:HG2	2.28	0.49
1:B:280:MET:O	1:B:281:MET:C	2.48	0.49
1:B:167:LEU:C	1:B:169:VAL:N	2.66	0.49
1:B:62:GLY:O	1:B:63:PRO:C	2.50	0.49
1:B:337:TYR:N	1:B:337:TYR:CD1	2.80	0.49
1:A:443:GLY:O	1:A:446:ALA:HB3	2.13	0.48
1:A:448:ARG:HH12	1:A:464:GLN:HB2	1.76	0.48
1:A:55:ASP:OD2	1:A:59:SER:CB	2.61	0.48
1:B:8:VAL:O	1:B:260:VAL:HA	2.12	0.48
1:B:28:LEU:HD13	1:B:454:MET:CE	2.42	0.48
1:B:392:GLN:HG2	1:B:393:TYR:CD1	2.48	0.48
1:A:346:ALA:O	1:A:347:HIS:C	2.50	0.48
1:B:79:THR:HG23	1:B:208:ARG:CB	2.44	0.48
1:A:171:LEU:HD22	1:A:171:LEU:O	2.14	0.48
1:A:426:THR:O	1:A:428:THR:N	2.46	0.48
1:B:437:GLU:O	1:B:438:GLY:C	2.52	0.48
1:B:215:GLY:O	1:B:219:GLU:HG2	2.13	0.48
1:A:42:ARG:CZ	2:A:600:FAD:H5'1	2.43	0.48
1:A:445:ARG:NE	1:A:449:GLU:OE2	2.45	0.48
1:A:270:MET:CG	1:A:286:ILE:CG2	2.84	0.48
1:B:75:LEU:HD21	1:B:221:ILE:HG12	1.94	0.48
1:A:240:GLN:NE2	1:A:421:ILE:HG13	2.28	0.48
1:A:438:GLY:O	1:A:440:VAL:N	2.46	0.48
1:A:413:VAL:O	1:A:413:VAL:CG1	2.61	0.48
2:A:600:FAD:O2'	2:A:600:FAD:H9	2.13	0.48
1:B:43:THR:CG2	1:B:43:THR:O	2.56	0.48
1:B:157:TRP:CE2	1:B:490:PRO:HG3	2.49	0.48
1:A:97:TYR:N	1:A:97:TYR:CD1	2.82	0.48
1:A:153:ASP:HA	1:A:162:LYS:HE2	1.95	0.48
1:B:280:MET:HG2	1:B:281:MET:N	2.27	0.48
1:A:246:LEU:CD2	1:A:256:GLU:HB3	2.44	0.48
1:A:215:GLY:O	1:A:216:GLN:C	2.51	0.48
1:A:320:GLU:OE2	1:A:347:HIS:NE2	2.47	0.48
1:A:385:GLU:O	1:A:385:GLU:HG3	2.13	0.48
1:B:138:PRO:O	1:B:139:LEU:HD23	2.13	0.48
1:A:42:ARG:NH2	2:A:600:FAD:O3P	2.42	0.48
1:A:6:ASP:CB	1:A:29:ASN:O	2.62	0.48
1:A:184:TRP:CZ2	1:A:401:TYR:HA	2.49	0.47
1:B:448:ARG:NH1	1:B:464:GLN:CB	2.70	0.47
1:B:448:ARG:HH12	1:B:464:GLN:HB2	1.75	0.47
1:A:362:LYS:O	1:A:366:GLU:HG3	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:THR:C	1:B:428:THR:N	2.63	0.47
1:B:4:LYS:HB2	1:B:256:GLU:HG3	1.96	0.47
1:A:65:GLN:CA	1:A:437:GLU:HG3	2.43	0.47
1:A:300:TYR:CE2	1:A:339:ALA:HB2	2.49	0.47
1:A:258:LYS:C	1:A:259:TYR:CG	2.87	0.47
1:A:250:LEU:HD21	1:B:237:TYR:CE1	2.49	0.47
1:A:206:GLN:NE2	3:A:601:NYP:H8N1	2.29	0.47
1:B:6:ASP:O	1:B:257:ALA:HB1	2.14	0.47
1:A:182:ALA:O	1:A:183:LEU:C	2.50	0.47
1:A:267:THR:HG22	1:B:270:MET:HE2	1.96	0.47
1:A:134:PRO:HG3	1:A:187:TRP:NE1	2.30	0.47
1:A:30:VAL:HG13	1:A:31:VAL:H	1.80	0.47
1:B:119:TRP:CE3	1:B:195:THR:HG21	2.50	0.47
1:A:135:TRP:CH2	1:A:412:ARG:HA	2.50	0.47
1:A:284:GLN:O	1:A:287:THR:HG22	2.15	0.47
1:A:28:LEU:CD1	1:A:454:MET:HE3	2.41	0.47
1:A:70:ARG:HG2	1:A:70:ARG:O	2.07	0.47
1:A:361:LEU:O	1:A:362:LYS:C	2.53	0.47
1:B:489:VAL:HB	1:B:490:PRO:HD3	1.96	0.47
1:B:114:ASP:O	1:B:115:HIS:C	2.52	0.47
1:B:184:TRP:CZ2	1:B:401:TYR:HA	2.48	0.47
1:A:413:VAL:O	1:A:414:LEU:C	2.54	0.47
1:A:485:HIS:O	1:A:486:LEU:C	2.50	0.47
1:B:270:MET:HG2	1:B:286:ILE:HG21	1.94	0.47
1:B:450:ILE:CG2	1:B:454:MET:HE2	2.45	0.47
1:A:137:ALA:O	1:A:138:PRO:C	2.51	0.47
1:B:413:VAL:O	1:B:413:VAL:CG1	2.63	0.47
1:A:444:GLU:HB3	1:A:448:ARG:HH21	1.80	0.47
1:A:249:THR:HG22	1:A:251:ASN:CB	2.43	0.47
1:A:69:LEU:O	1:A:72:ALA:HB3	2.15	0.47
1:A:355:LEU:HB3	1:A:359:GLU:HB2	1.97	0.47
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.62	0.47
1:A:270:MET:CG	1:A:286:ILE:HG22	2.46	0.46
1:B:194:GLY:O	1:B:195:THR:C	2.53	0.46
1:B:358:GLU:H	1:B:358:GLU:HG2	1.33	0.46
1:A:171:LEU:CD2	1:A:171:LEU:O	2.63	0.46
1:A:291:LEU:CD2	1:A:399:THR:O	2.64	0.46
1:B:282:ARG:CZ	1:B:423:PHE:CZ	2.99	0.46
1:B:407:LEU:HA	1:B:407:LEU:HD12	1.32	0.46
1:B:446:ALA:O	1:B:449:GLU:HB2	2.15	0.46
1:B:381:VAL:O	1:B:381:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:HB2	1:A:280:MET:HE2	1.60	0.46
1:A:298:ILE:N	1:A:298:ILE:HD12	2.30	0.46
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.64	0.46
1:B:171:LEU:HA	1:B:345:LEU:CD1	2.45	0.46
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.62	0.46
1:B:387:ASN:OD1	1:B:387:ASN:C	2.53	0.46
1:B:233:ARG:HD2	1:B:251:ASN:HD22	1.80	0.46
1:B:285:MET:C	1:B:287:THR:N	2.68	0.46
1:A:191:GLN:NE2	1:A:433:SER:HB3	2.31	0.46
1:B:275:ASN:OD1	1:B:276:PRO:HA	2.16	0.46
1:B:196:THR:O	1:B:197:ARG:C	2.53	0.46
1:B:375:LEU:O	1:B:376:GLU:C	2.52	0.46
1:B:97:TYR:CD1	1:B:97:TYR:N	2.84	0.46
1:B:168:PHE:CD1	1:B:168:PHE:O	2.69	0.46
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.79	0.46
1:A:440:VAL:O	1:A:441:GLU:C	2.53	0.46
1:B:184:TRP:O	1:B:187:TRP:HB3	2.16	0.46
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.22	0.46
1:A:17:MET:O	1:A:18:ALA:C	2.53	0.46
3:A:601:NYP:H6	3:A:601:NYP:H8N1	1.97	0.46
1:A:320:GLU:C	1:A:322:ALA:N	2.69	0.46
1:A:61:VAL:O	1:A:61:VAL:HG12	2.14	0.46
1:B:236:ILE:HD11	1:B:250:LEU:CD1	2.28	0.46
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.51	0.46
1:B:233:ARG:HD3	1:B:233:ARG:HA	1.66	0.46
1:A:320:GLU:O	1:A:322:ALA:N	2.49	0.46
1:A:9:VAL:HG22	1:A:261:ILE:HB	1.98	0.46
1:B:174:THR:HG22	1:B:292:GLY:CA	2.46	0.45
1:B:174:THR:HG22	1:B:293:SER:N	2.20	0.45
1:A:113:LEU:CD2	1:A:486:LEU:HB3	2.46	0.45
1:A:167:LEU:C	1:A:169:VAL:N	2.69	0.45
1:A:451:LEU:CB	1:A:457:ILE:HD12	2.44	0.45
1:B:275:ASN:CA	1:B:276:PRO:C	2.84	0.45
1:A:198:ILE:CG2	1:A:199:ILE:N	2.79	0.45
1:B:480:THR:O	1:B:484:ARG:HG2	2.16	0.45
1:A:80:TYR:CG	1:A:80:TYR:O	2.70	0.45
1:B:174:THR:CG2	1:B:292:GLY:HA3	2.46	0.45
1:B:75:LEU:H	1:B:75:LEU:HD12	1.81	0.45
1:A:189:VAL:HG12	1:A:194:GLY:HA2	1.99	0.45
1:B:167:LEU:O	1:B:169:VAL:N	2.49	0.45
1:A:178:HIS:CG	1:B:145:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:HA	1:A:105:PRO:HD3	1.86	0.45
1:A:358:GLU:HG2	1:A:358:GLU:H	1.21	0.45
1:A:280:MET:HB3	1:A:280:MET:HE3	1.68	0.45
1:A:343:PHE:HB3	1:A:345:LEU:CD2	2.46	0.45
1:B:86:GLU:CD	1:B:86:GLU:H	2.19	0.45
1:A:143:TRP:HA	1:A:146:MET:HE3	1.96	0.45
1:A:23:LEU:O	1:A:26:SER:CB	2.64	0.45
1:B:375:LEU:HA	1:B:375:LEU:HD23	1.65	0.45
1:A:173:VAL:HG21	1:A:184:TRP:CZ3	2.51	0.45
1:A:457:ILE:HA	1:A:458:PRO:HD3	1.81	0.45
1:B:456:LYS:HB3	1:B:456:LYS:HE2	1.85	0.45
1:A:188:TYR:O	1:A:189:VAL:C	2.55	0.45
1:A:86:GLU:N	1:A:86:GLU:CD	2.66	0.45
1:B:30:VAL:HG13	1:B:31:VAL:N	2.31	0.45
1:B:137:ALA:O	1:B:138:PRO:C	2.55	0.45
1:B:207:GLU:HG2	1:B:208:ARG:HG2	1.98	0.45
1:A:489:VAL:O	1:A:493:LEU:HG	2.16	0.45
1:B:291:LEU:HD22	1:B:399:THR:O	2.17	0.45
1:B:41:GLY:H	1:B:43:THR:HG22	1.82	0.45
1:B:134:PRO:HD2	1:B:135:TRP:CE3	2.51	0.45
1:A:216:GLN:CA	1:A:219:GLU:HG3	2.46	0.45
1:A:164:LEU:HD12	1:A:164:LEU:O	2.17	0.45
1:A:498:LEU:O	1:A:498:LEU:HD12	2.17	0.45
1:B:79:THR:CG2	1:B:208:ARG:HH11	2.27	0.45
1:A:42:ARG:HB3	2:A:600:FAD:C8M	2.47	0.45
1:A:480:THR:CB	1:A:483:GLU:HB2	2.24	0.45
1:A:169:VAL:O	1:A:170:ASN:C	2.54	0.45
1:B:442:ALA:O	1:B:445:ARG:N	2.50	0.45
1:B:109:PRO:C	1:B:111:THR:H	2.19	0.45
1:B:168:PHE:CE1	1:B:199:ILE:HD11	2.52	0.45
1:A:134:PRO:HD2	1:A:135:TRP:CZ3	2.52	0.44
1:B:457:ILE:HG23	1:B:458:PRO:HD2	1.99	0.44
1:B:86:GLU:HG2	1:B:312:CYS:HB3	1.99	0.44
1:A:387:ASN:OD1	1:A:389:CYS:HB2	2.17	0.44
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.63	0.44
1:B:291:LEU:HD23	1:B:400:THR:CA	2.45	0.44
1:A:191:GLN:NE2	1:A:433:SER:H	2.14	0.44
1:B:144:ASP:OD2	1:B:408:THR:CB	2.59	0.44
1:A:298:ILE:HG21	1:A:300:TYR:CZ	2.52	0.44
1:A:450:ILE:CG2	1:A:454:MET:HE2	2.48	0.44
1:B:457:ILE:HG23	1:B:461:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLU:HG2	1:B:312:CYS:CA	2.47	0.44
1:A:168:PHE:CD1	1:A:199:ILE:HD11	2.52	0.44
1:B:119:TRP:O	1:B:120:ARG:C	2.54	0.44
1:A:159:GLU:O	1:A:160:SER:C	2.55	0.44
1:B:202:THR:HG22	1:B:203:ASN:N	2.31	0.44
1:A:280:MET:HG2	1:A:281:MET:N	2.32	0.44
1:B:445:ARG:CD	1:B:463:TRP:CZ2	2.99	0.44
1:B:151:LEU:O	1:B:152:LEU:C	2.54	0.44
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.42	0.44
1:B:79:THR:HG22	1:B:80:TYR:N	2.32	0.44
1:B:236:ILE:CG2	1:B:236:ILE:O	2.63	0.44
1:B:216:GLN:O	1:B:217:VAL:C	2.55	0.44
1:A:191:GLN:NE2	1:A:433:SER:O	2.51	0.44
1:B:119:TRP:CE3	1:B:195:THR:CG2	3.00	0.44
1:A:303:GLU:CB	1:A:304:PRO:HD2	2.48	0.44
1:A:300:TYR:HD2	1:A:339:ALA:HB2	1.79	0.44
1:A:157:TRP:CE2	1:A:490:PRO:HG3	2.52	0.44
1:B:285:MET:HE2	1:B:414:LEU:HD23	2.00	0.44
1:A:388:TRP:O	1:A:389:CYS:C	2.55	0.44
1:A:285:MET:HE1	1:A:414:LEU:HA	2.00	0.44
1:A:54:VAL:HG13	1:A:300:TYR:HH	1.82	0.44
1:A:6:ASP:HB2	1:A:29:ASN:HB2	1.99	0.44
1:A:249:THR:CG2	1:A:251:ASN:CB	2.93	0.44
1:A:270:MET:HE1	1:B:267:THR:HG22	2.00	0.44
1:A:468:GLU:OE2	1:A:473:PRO:HA	2.17	0.44
1:A:86:GLU:HB2	1:A:311:TYR:C	2.38	0.44
1:A:282:ARG:CZ	1:A:423:PHE:CZ	3.01	0.44
1:A:239:ASP:OD1	1:A:239:ASP:C	2.56	0.44
1:A:480:THR:HG22	1:A:482:LEU:H	1.83	0.44
1:B:249:THR:O	1:B:252:HIS:N	2.42	0.44
1:B:378:LEU:HD22	1:B:378:LEU:HA	1.83	0.44
1:A:145:ASN:OD1	1:B:178:HIS:CE1	2.71	0.44
1:A:304:PRO:O	1:A:307:ARG:HD2	2.17	0.43
1:A:287:THR:CG2	1:A:288:ARG:HG3	2.46	0.43
1:A:445:ARG:CD	1:A:463:TRP:CH2	3.00	0.43
1:A:202:THR:HG22	1:A:203:ASN:N	2.33	0.43
1:B:471:ASP:C	1:B:473:PRO:HD3	2.37	0.43
1:A:381:VAL:O	1:A:382:HIS:HB2	2.18	0.43
1:B:191:GLN:NE2	1:B:433:SER:HB3	2.32	0.43
3:A:601:NYP:C8N	3:A:601:NYP:H6	2.49	0.43
1:A:75:LEU:HD21	1:A:221:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:VAL:O	1:B:421:ILE:HA	2.18	0.43
1:B:184:TRP:O	1:B:185:PHE:C	2.55	0.43
1:B:66:ASN:ND2	1:B:468:GLU:HA	2.33	0.43
1:A:207:GLU:HG2	1:A:208:ARG:HG2	1.99	0.43
1:A:295:ILE:HG22	1:A:297:CYS:SG	2.58	0.43
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.77	0.43
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.67	0.43
1:A:184:TRP:O	1:A:187:TRP:HB3	2.17	0.43
1:A:443:GLY:O	1:A:444:GLU:C	2.55	0.43
1:A:471:ASP:C	1:A:473:PRO:HD3	2.39	0.43
1:A:146:MET:HB2	1:A:146:MET:HE2	1.85	0.43
1:A:79:THR:CG2	1:A:208:ARG:HH11	2.24	0.43
1:A:42:ARG:HA	1:A:388:TRP:CZ3	2.54	0.43
1:A:362:LYS:HG2	1:A:366:GLU:OE2	2.19	0.43
1:B:241:THR:HG22	1:B:242:ARG:N	2.32	0.43
1:A:23:LEU:HA	1:A:23:LEU:HD23	1.84	0.43
1:A:23:LEU:O	1:A:26:SER:N	2.49	0.43
1:A:35:ALA:HB1	1:A:234:PRO:HG3	2.00	0.43
1:B:79:THR:CG2	1:B:80:TYR:N	2.81	0.43
1:A:171:LEU:CD1	3:A:601:NYP:C2	2.90	0.43
1:A:70:ARG:NH2	1:A:444:GLU:OE2	2.51	0.43
1:A:264:ILE:HG21	1:A:268:LEU:C	2.39	0.43
1:A:161:ALA:O	1:A:162:LYS:C	2.56	0.43
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.59	0.43
1:B:79:THR:HG23	1:B:208:ARG:HB3	1.99	0.43
1:B:344:ILE:HG22	1:B:349:ALA:HA	2.01	0.43
1:A:438:GLY:O	1:A:441:GLU:N	2.52	0.43
1:A:157:TRP:CZ2	1:A:490:PRO:HG3	2.54	0.43
1:A:49:GLN:CG	1:A:50:LYS:N	2.74	0.43
1:B:86:GLU:N	1:B:86:GLU:CD	2.69	0.43
1:B:61:VAL:HG12	1:B:61:VAL:O	2.17	0.43
1:B:258:LYS:C	1:B:259:TYR:CG	2.90	0.43
1:A:331:THR:OG1	1:A:338:ALA:HA	2.19	0.43
1:B:480:THR:HG22	1:B:482:LEU:H	1.83	0.42
1:A:442:ALA:O	1:A:443:GLY:C	2.56	0.42
1:A:267:THR:O	1:A:267:THR:HG22	2.18	0.42
1:B:430:THR:HG22	1:B:430:THR:O	2.19	0.42
1:A:332:LYS:HD3	1:A:332:LYS:HA	1.78	0.42
1:A:480:THR:O	1:A:484:ARG:HG2	2.19	0.42
1:A:346:ALA:O	1:A:349:ALA:N	2.52	0.42
1:A:235:VAL:CG1	1:A:236:ILE:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HD12	1:B:250:LEU:HA	2.01	0.42
1:A:459:GLU:O	1:A:460:ASP:C	2.57	0.42
1:A:252:HIS:HE1	1:B:248:GLU:OE2	2.00	0.42
1:A:117:ASN:O	1:A:118:PHE:C	2.56	0.42
1:B:171:LEU:HD11	3:B:601:NYP:H2	2.02	0.42
1:B:38:ARG:HH11	1:B:38:ARG:HD3	1.65	0.42
1:B:28:LEU:CD1	1:B:454:MET:CE	2.98	0.42
1:A:374:SER:O	1:A:375:LEU:C	2.56	0.42
1:A:377:ALA:C	1:A:379:GLU:H	2.23	0.42
1:A:264:ILE:O	1:A:265:PRO:C	2.57	0.42
1:B:286:ILE:CG2	1:B:286:ILE:O	2.65	0.42
1:A:270:MET:CE	1:B:267:THR:HG22	2.49	0.42
1:B:445:ARG:HD3	1:B:463:TRP:CH2	2.54	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.47	0.42
1:B:314:THR:HA	1:B:327:THR:O	2.20	0.42
1:B:317:ILE:HD13	1:B:371:VAL:HG21	2.01	0.42
1:B:427:GLU:H	1:B:427:GLU:HG2	1.10	0.42
1:B:51:VAL:HG22	1:B:300:TYR:CE1	2.55	0.42
1:B:46:LEU:HB3	1:B:54:VAL:HG23	2.02	0.42
1:B:23:LEU:O	1:B:26:SER:CB	2.68	0.42
1:B:236:ILE:HG21	1:B:236:ILE:HD13	1.65	0.42
1:A:457:ILE:HG23	1:A:461:GLU:HB2	2.02	0.42
1:A:70:ARG:HH22	1:A:444:GLU:CD	2.22	0.42
1:B:286:ILE:HG21	1:B:286:ILE:HD13	1.50	0.42
1:B:88:LEU:O	1:B:98:PRO:HA	2.20	0.42
1:B:219:GLU:H	1:B:219:GLU:HG2	1.56	0.42
1:B:426:THR:O	1:B:428:THR:N	2.53	0.42
1:A:55:ASP:OD2	1:A:59:SER:HB2	2.20	0.42
1:B:332:LYS:HB3	1:B:333:PRO:HD2	2.02	0.42
1:B:139:LEU:O	1:B:140:ALA:C	2.58	0.42
1:A:79:THR:HG23	1:A:208:ARG:CB	2.49	0.42
1:A:313:GLY:O	1:A:327:THR:HG23	2.20	0.42
1:B:457:ILE:HA	1:B:458:PRO:HD3	1.83	0.42
1:A:143:TRP:O	1:A:182:ALA:HB3	2.19	0.42
1:A:411:GLY:C	1:A:413:VAL:H	2.24	0.41
1:A:171:LEU:CD2	1:A:171:LEU:C	2.88	0.41
1:B:341:MET:HE2	1:B:341:MET:HB3	1.83	0.41
1:A:115:HIS:O	1:A:116:ASN:C	2.57	0.41
1:B:119:TRP:HE3	1:B:195:THR:HG21	1.86	0.41
1:A:445:ARG:HH11	1:A:445:ARG:HD3	1.68	0.41
1:A:181:SER:O	1:A:182:ALA:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HG3	1:A:437:GLU:OE2	2.21	0.41
1:A:237:TYR:CE1	1:B:250:LEU:HD21	2.56	0.41
1:A:267:THR:HG21	1:B:287:THR:OG1	2.21	0.41
1:A:275:ASN:CA	1:A:276:PRO:C	2.87	0.41
1:B:147:THR:O	1:B:148:MET:C	2.56	0.41
1:B:355:LEU:HB3	1:B:359:GLU:HB2	2.02	0.41
1:B:303:GLU:HB3	1:B:304:PRO:CD	2.48	0.41
1:B:490:PRO:O	1:B:491:GLY:C	2.58	0.41
1:B:195:THR:O	1:B:196:THR:C	2.58	0.41
1:B:416:GLN:HA	1:B:417:PRO:HD3	1.81	0.41
1:A:402:PHE:HZ	1:A:414:LEU:HD11	1.84	0.41
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.94	0.41
1:A:84:GLU:OE2	1:A:201:THR:HB	2.20	0.41
1:B:266:PRO:O	1:B:267:THR:C	2.57	0.41
1:B:303:GLU:HB3	1:B:304:PRO:HD3	2.03	0.41
1:A:151:LEU:HD12	1:A:151:LEU:O	2.21	0.41
1:B:365:CYS:O	1:B:366:GLU:C	2.59	0.41
1:B:141:GLU:O	1:B:142:GLU:C	2.56	0.41
1:A:79:THR:HG23	1:A:208:ARG:HB3	2.03	0.41
1:B:388:TRP:O	1:B:390:GLU:N	2.53	0.41
1:A:41:GLY:HA3	2:A:600:FAD:O2A	2.21	0.41
1:A:250:LEU:HD21	1:B:237:TYR:CD1	2.55	0.41
1:A:165:ALA:O	1:A:168:PHE:HB3	2.20	0.41
1:A:184:TRP:O	1:A:185:PHE:C	2.55	0.41
1:A:388:TRP:C	1:A:390:GLU:N	2.74	0.41
1:B:191:GLN:HE22	1:B:433:SER:CA	2.33	0.41
1:A:167:LEU:O	1:A:169:VAL:N	2.54	0.41
1:B:42:ARG:NH2	2:B:600:FAD:O3P	2.53	0.41
1:A:165:ALA:O	1:A:166:THR:C	2.58	0.41
1:A:103:PHE:HA	1:A:104:PRO:HD3	1.75	0.41
1:B:97:TYR:HA	1:B:98:PRO:HD3	1.70	0.41
1:A:304:PRO:HB2	1:A:307:ARG:HD3	1.93	0.41
1:A:174:THR:HG22	1:A:292:GLY:HA3	1.91	0.41
1:B:451:LEU:HB3	1:B:457:ILE:HD12	2.02	0.41
1:B:92:VAL:CG1	1:B:93:LYS:N	2.84	0.41
1:A:89:ILE:HG21	1:A:96:SER:HB3	2.01	0.41
1:A:373:GLY:C	1:A:374:SER:OG	2.59	0.41
1:A:437:GLU:O	1:A:438:GLY:C	2.58	0.41
1:B:480:THR:CB	1:B:483:GLU:HB2	2.23	0.41
1:A:169:VAL:C	1:A:171:LEU:N	2.72	0.41
1:B:233:ARG:NH1	1:B:253:GLU:CD	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:O	1:B:283:ASN:C	2.59	0.41
1:B:413:VAL:O	1:B:414:LEU:C	2.58	0.41
1:A:286:ILE:HD13	1:A:286:ILE:HG21	1.64	0.41
1:A:71:LEU:O	1:A:72:ALA:C	2.58	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.75	0.41
1:A:418:VAL:O	1:A:418:VAL:HG12	2.20	0.41
1:A:245:VAL:O	1:A:256:GLU:HA	2.21	0.41
1:A:108:ASN:O	1:A:112:TYR:N	2.54	0.41
1:B:245:VAL:HG23	1:B:257:ALA:O	2.21	0.41
1:A:16:GLY:O	1:A:20:ALA:N	2.40	0.41
1:A:148:MET:HB3	1:A:148:MET:HE2	1.95	0.41
1:A:392:GLN:O	1:A:392:GLN:HG3	2.20	0.41
1:B:161:ALA:O	1:B:162:LYS:C	2.58	0.41
1:A:225:LEU:HA	1:A:225:LEU:HD23	1.62	0.41
1:A:242:ARG:HB3	1:A:243:GLU:H	1.67	0.41
1:A:92:VAL:HG12	1:A:93:LYS:HG3	2.03	0.41
1:B:174:THR:HG22	1:B:174:THR:O	2.17	0.40
1:A:271:LYS:HA	1:A:271:LYS:HD3	1.95	0.40
1:A:375:LEU:O	1:A:376:GLU:C	2.57	0.40
1:B:39:VAL:HG13	1:B:39:VAL:O	2.21	0.40
1:B:304:PRO:O	1:B:305:PHE:C	2.59	0.40
1:A:75:LEU:CD2	1:A:221:ILE:HG12	2.51	0.40
1:A:344:ILE:HG22	1:A:349:ALA:HA	2.04	0.40
1:A:254:MET:HB3	1:A:254:MET:HE3	1.72	0.40
1:A:436:MET:O	1:A:437:GLU:C	2.59	0.40
1:B:411:GLY:C	1:B:413:VAL:H	2.23	0.40
1:A:235:VAL:HG12	1:A:236:ILE:N	2.30	0.40
1:A:450:ILE:O	1:A:451:LEU:C	2.60	0.40
1:A:252:HIS:ND1	1:B:252:HIS:ND1	2.69	0.40
1:A:108:ASN:O	1:A:111:THR:HB	2.22	0.40
1:A:407:LEU:O	1:A:411:GLY:HA3	2.20	0.40
1:A:175:ALA:CB	1:A:179:GLU:OE1	2.47	0.40
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.51	0.40
1:B:126:GLY:O	1:B:128:GLU:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/520 (95%)	391 (79%)	83 (17%)	21 (4%)	3	20
1	B	491/520 (94%)	400 (82%)	76 (16%)	15 (3%)	5	28
All	All	986/1040 (95%)	791 (80%)	159 (16%)	36 (4%)	4	23

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	CYS
1	B	286	ILE
1	B	442	ALA
1	B	446	ALA
1	A	252	HIS
1	A	286	ILE
1	A	398	TYR
1	A	446	ALA
1	A	496	ILE
1	B	132	ASP
1	B	195	THR
1	B	252	HIS
1	A	122	MET
1	A	132	ASP
1	A	321	GLU
1	A	365	CYS
1	A	408	THR
1	B	398	TYR
1	A	419	ASP
1	A	442	ALA
1	B	212	GLY
1	B	365	CYS
1	B	408	THR
1	B	412	ARG
1	A	86	GLU

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Mol	Chain	Res	Type
1	A	127	ARG
1	A	382	HIS
1	A	404	PRO
1	A	412	ARG
1	B	110	ILE
1	B	419	ASP
1	A	336	ASN
1	B	114	ASP
1	B	389	CYS
1	A	41	GLY
1	A	39	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/444 (96%)	353 (83%)	73 (17%)	2	12
1	B	423/444 (95%)	343 (81%)	80 (19%)	2	10
All	All	849/888 (96%)	696 (82%)	153 (18%)	2	11

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	ASP
1	A	22	LEU
1	A	38	ARG
1	A	39	VAL
1	A	43	THR
1	A	48	ASN
1	A	49	GLN
1	A	54	VAL
1	A	61	VAL
1	A	64	THR
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	81	LYS
1	A	86	GLU
1	A	88	LEU
1	A	107	TRP
1	A	128	GLU
1	A	131	SER
1	A	147	THR
1	A	155	LEU
1	A	160	SER
1	A	171	LEU
1	A	174	THR
1	A	180	VAL
1	A	181	SER
1	A	190	LYS
1	A	195	THR
1	A	198	ILE
1	A	201	THR
1	A	208	ARG
1	A	219	GLU
1	A	232	GLU
1	A	233	ARG
1	A	236	ILE
1	A	243	GLU
1	A	254	MET
1	A	256	GLU
1	A	262	SER
1	A	271	LYS
1	A	280	MET
1	A	282	ARG
1	A	287	THR
1	A	303	GLU
1	A	306	TRP
1	A	327	THR
1	A	354	ARG
1	A	356	THR
1	A	361	LEU
1	A	374	SER
1	A	378	LEU
1	A	381	VAL
1	A	397	CYS
1	A	398	TYR

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Mol	Chain	Res	Type
1	A	399	THR
1	A	404	PRO
1	A	412	ARG
1	A	416	GLN
1	A	427	GLU
1	A	428	THR
1	A	437	GLU
1	A	456	LYS
1	A	462	ILE
1	A	465	SER
1	A	466	GLU
1	A	469	SER
1	A	471	ASP
1	A	472	VAL
1	A	477	ILE
1	A	479	THR
1	A	495	LEU
1	A	498	LEU
1	A	500	THR
1	B	4	LYS
1	B	6	ASP
1	B	22	LEU
1	B	26	SER
1	B	38	ARG
1	B	39	VAL
1	B	43	THR
1	B	47	ARG
1	B	48	ASN
1	B	49	GLN
1	B	54	VAL
1	B	61	VAL
1	B	64	THR
1	B	69	LEU
1	B	73	LYS
1	B	84	GLU
1	B	86	GLU
1	B	88	LEU
1	B	107	TRP
1	B	128	GLU
1	B	131	SER
1	B	147	THR
1	B	155	LEU

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Mol	Chain	Res	Type
1	B	160	SER
1	B	171	LEU
1	B	174	THR
1	B	180	VAL
1	B	181	SER
1	B	190	LYS
1	B	195	THR
1	B	198	ILE
1	B	201	THR
1	B	202	THR
1	B	219	GLU
1	B	232	GLU
1	B	233	ARG
1	B	236	ILE
1	B	241	THR
1	B	243	GLU
1	B	254	MET
1	B	256	GLU
1	B	262	SER
1	B	271	LYS
1	B	280	MET
1	B	282	ARG
1	B	287	THR
1	B	303	GLU
1	B	306	TRP
1	B	327	THR
1	B	337	TYR
1	B	341	MET
1	B	351	LYS
1	B	354	ARG
1	B	356	THR
1	B	361	LEU
1	B	364	LEU
1	B	370	LYS
1	B	374	SER
1	B	378	LEU
1	B	381	VAL
1	B	397	CYS
1	B	398	TYR
1	B	399	THR
1	B	408	THR
1	B	412	ARG

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Mol	Chain	Res	Type
1	B	416	GLN
1	B	427	GLU
1	B	428	THR
1	B	437	GLU
1	B	441	GLU
1	B	456	LYS
1	B	462	ILE
1	B	465	SER
1	B	466	GLU
1	B	469	SER
1	B	471	ASP
1	B	477	ILE
1	B	478	THR
1	B	479	THR
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	83	ASN
1	A	90	HIS
1	A	116	ASN
1	A	178	HIS
1	A	191	GLN
1	A	206	GLN
1	A	216	GLN
1	A	251	ASN
1	A	431	HIS
1	A	485	HIS
1	B	24	HIS
1	B	116	ASN
1	B	178	HIS
1	B	206	GLN
1	B	251	ASN
1	B	431	HIS
1	B	485	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	600	1,3	48,58,58	1.37	7 (14%)	54,89,89	2.65	13 (24%)
3	NYP	A	601	2	9,12,12	4.03	8 (88%)	11,14,14	3.84	8 (72%)
2	FAD	B	600	1,3	48,58,58	1.34	5 (10%)	54,89,89	2.49	14 (25%)
3	NYP	B	601	2	9,12,12	4.12	8 (88%)	11,14,14	3.59	7 (63%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1,3	-	0/30/50/50	0/6/6/6
3	NYP	A	601	2	1/1/2/6	0/4/15/15	0/1/1/1
2	FAD	B	600	1,3	-	0/30/50/50	0/6/6/6
3	NYP	B	601	2	1/1/2/6	0/4/15/15	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NYP	C6-C1	-6.68	1.38	1.52
3	B	601	NYP	C6-C1	-6.20	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NYP	C2-C3	-5.21	1.40	1.52
3	B	601	NYP	C2-C3	-5.00	1.40	1.52
3	A	601	NYP	C2-C1	-4.94	1.39	1.52
3	B	601	NYP	C2-C1	-4.38	1.40	1.52
3	A	601	NYP	C6-C5	-3.98	1.40	1.49
3	B	601	NYP	C6-C5	-3.87	1.40	1.49
2	A	600	FAD	C10-N10	-2.42	1.36	1.39
3	A	601	NYP	C3-C4	-2.23	1.40	1.48
2	A	600	FAD	C6-C5X	-2.16	1.38	1.41
2	B	600	FAD	C10-N10	-2.14	1.36	1.39
3	B	601	NYP	C3-C4	-2.12	1.41	1.48
2	A	600	FAD	C9A-C5X	-2.11	1.38	1.42
2	B	600	FAD	C2A-N1A	2.35	1.38	1.33
2	A	600	FAD	C4-N3	2.64	1.38	1.33
3	B	601	NYP	C9-C10	2.68	1.50	1.42
3	A	601	NYP	C5-C4	2.69	1.39	1.32
3	A	601	NYP	C9-C10	2.69	1.50	1.42
2	A	600	FAD	C2A-N1A	2.72	1.39	1.33
2	B	600	FAD	C4-N3	2.87	1.38	1.33
2	A	600	FAD	C4X-N5	3.00	1.38	1.33
3	B	601	NYP	C5-C4	3.06	1.40	1.32
2	B	600	FAD	C4X-N5	3.07	1.38	1.33
2	A	600	FAD	C2A-N3A	3.77	1.38	1.32
3	A	601	NYP	C9-N8	3.86	1.32	1.30
2	B	600	FAD	C2A-N3A	4.08	1.39	1.32
3	B	601	NYP	C9-N8	5.82	1.33	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-10.10	121.16	128.89
2	A	600	FAD	P-O3P-PA	-9.93	104.85	132.73
2	B	600	FAD	P-O3P-PA	-8.39	109.17	132.73
2	B	600	FAD	N3A-C2A-N1A	-8.25	122.58	128.89
2	A	600	FAD	C4X-C10-N10	-4.23	118.03	120.52
3	A	601	NYP	C11-C10-C9	-4.05	116.85	122.69
2	B	600	FAD	C4X-C10-N10	-3.77	118.30	120.52
2	A	600	FAD	C9A-C5X-N5	-3.55	117.10	122.36
2	A	600	FAD	O3'-C3'-C2'	-3.46	100.04	108.75
3	B	601	NYP	C11-C10-C9	-3.38	117.82	122.69
2	B	600	FAD	C9A-C5X-N5	-3.31	117.46	122.36
2	B	600	FAD	C4X-C4-N3	-3.06	119.40	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O3'-C3'-C2'	-2.95	101.31	108.75
2	B	600	FAD	C7M-C7-C8	-2.87	114.43	120.73
2	A	600	FAD	C4X-C4-N3	-2.56	120.09	123.59
3	A	601	NYP	C7-N8-C9	-2.24	116.62	121.52
2	A	600	FAD	C5B-C4B-C3B	-2.21	106.42	115.21
2	A	600	FAD	O3P-P-O5'	-2.12	97.32	102.94
2	A	600	FAD	C7-C6-C5X	-2.03	117.61	120.92
2	B	600	FAD	C4X-N5-C5X	2.25	119.35	116.76
2	B	600	FAD	C1B-N9A-C4A	2.36	130.50	126.94
2	B	600	FAD	C4-C4X-N5	2.52	121.77	118.72
3	B	601	NYP	C8N-N8-C7	2.62	123.26	115.04
3	B	601	NYP	C2-C3-C4	2.76	118.40	112.30
2	B	600	FAD	N6A-C6A-N1A	2.83	125.28	119.20
3	A	601	NYP	C8N-N8-C7	3.01	124.48	115.04
2	B	600	FAD	C5X-C9A-N10	3.02	119.91	117.62
2	A	600	FAD	O5'-P-O1P	3.06	121.51	109.62
3	B	601	NYP	C2-C1-C7	3.16	118.18	111.23
2	B	600	FAD	C4B-O4B-C1B	3.34	113.39	109.72
3	A	601	NYP	C2-C1-C7	3.41	118.72	111.23
2	A	600	FAD	O2P-P-O3P	3.42	120.60	105.09
3	A	601	NYP	C2-C3-C4	3.60	120.28	112.30
3	A	601	NYP	C3-C2-C1	4.26	119.56	112.64
3	B	601	NYP	C3-C2-C1	4.57	120.06	112.64
2	A	600	FAD	C4-N3-C2	5.01	119.58	115.25
3	B	601	NYP	C1-C6-C5	5.24	118.78	113.00
2	A	600	FAD	C5X-C9A-N10	5.58	121.86	117.62
3	A	601	NYP	C1-C6-C5	6.37	120.03	113.00
3	A	601	NYP	C2-C1-C6	6.55	120.67	109.63
2	B	600	FAD	C4-N3-C2	6.77	121.10	115.25
3	B	601	NYP	C2-C1-C6	7.05	121.52	109.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	NYP	C1
3	A	601	NYP	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	7	0
3	A	601	NYP	12	0
2	B	600	FAD	3	0
3	B	601	NYP	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	497/520 (95%)	-0.13	4 (0%) 87 67	27, 44, 74, 100	0
1	B	493/520 (94%)	-0.38	2 (0%) 93 80	27, 44, 73, 91	0
All	All	990/1040 (95%)	-0.26	6 (0%) 90 73	27, 44, 74, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	3.0
1	B	243	GLU	2.8
1	A	27	GLY	2.8
1	B	107	TRP	2.2
1	A	4	LYS	2.1
1	A	302	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NYP	A	601	12/12	0.87	0.27	3.88	46,53,58,59	0
3	NYP	B	601	12/12	0.91	0.21	1.23	46,53,58,58	0
2	FAD	A	600	53/53	0.90	0.21	-0.11	24,35,45,49	0
2	FAD	B	600	53/53	0.96	0.14	-1.05	23,35,45,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.